



Hemoglobin Calibration Curves by Photoacoustic Spectroscopy

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Abstract

In the present study, hemoglobin calibration curves were developed by photoacoustic spectroscopy (PAS) using hemoglobin solutions with controlled concentrations. Two types of samples exhibiting different optical properties were obtained: optically opaque (20–180 mg/mL concentrations) and optically transparent (0.0312–2 mg/mL concentrations). Optical absorption spectra were recorded in the wavelength range of 250–750 nm. From these spectra, the Soret band absorption peak at 412 nm and a secondary absorption at 450 nm were identified, and their ratio was determined. The ratios, plotted as a function of hemoglobin concentration, were fitted to the most suitable mathematical model, enabling the estimation of unknown hemoglobin concentrations in various biological samples, both optically opaque (e.g., blood and organs) and optically transparent (e.g., urine and plasma). The results show a strong correlation between the photoacoustic signal and hemoglobin concentration, validating the applicability of this technique to complex biological systems. Accurate quantification of hemoglobin in biological media is essential for the diagnosis and monitoring of numerous diseases. PAS proves to be a reliable tool for clinical and biomedical research applications, offering advantages in sensitivity, specificity, and minimal sample volume requirements.

Keywords Biomedical applications · Hemoglobin calibration curves · Optical absorption · Photoacoustic spectroscopy

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1 Introduction

Red blood cells are primarily composed of hemoglobin; a complex protein whose main function is to transport oxygen from the lungs to the tissues and to carry carbon dioxide from the tissues back to the lungs for elimination [1–3]. Given its importance in metabolism and the regulation of vital functions, accurate monitoring of hemoglobin levels is essential in the diagnosis and treatment of several diseases[4], such as anemia [5], cardiovascular diseases [6], and even septic shock [5, 7, 8]. Conventional methods for measuring hemoglobin concentrations in biological samples include optical absorption spectrophotometry and chromatography [9, 10], which, although effective, have limitations when it comes to measuring in complex biological media such as human tissues, where the effects of light scattering and absorption can alter the results, and large amounts of sample need to be extracted for analysis, making them not viable for constant and continuous monitoring of hemoglobin concentrations [11].

In this context, Photoacoustic Spectroscopy (PAS) has emerged as a reliable technique for the quantitative measurement of biomolecules in biological media [12–20]. PAS integrates the advantages of optical and acoustic spectroscopy by generating photoacoustic signals resulting from light absorption by molecules [21, 22]. In essence, when a biological material, such as hemoglobin, absorbs modulated light, the absorbed energy induces periodic thermal fluctuations that produce pressure variations in the medium surrounding the sample [23]. These pressure variations propagate as acoustic waves, which can then be detected and analyzed [24]. This phenomenon, known as the photoacoustic effect [25], enables PAS to overcome many limitations of conventional optical techniques, providing high sensitivity and molecular specificity even in highly scattering tissues. Furthermore, PAS is a noninvasive and non-destructive technique that requires only microliter-scale sample volumes, making it particularly suitable for studying biological systems [12–20].

Unlike other optical techniques that rely solely on measuring the intensity of absorbed or transmitted light [26], Photoacoustic Spectroscopy generates a signal directly proportional to hemoglobin concentration, making it a powerful tool for accurate hemoglobin quantification [17, 27]. PAS can detect small variations in hemoglobin levels, which makes it particularly suitable for biomedical studies requiring high sensitivity and precision [17, 28]. However, to achieve reliable quantitative results, it is essential to establish calibration curves that correlate the intensity of the photoacoustic signal with the hemoglobin concentration in biological samples.

The present study aims to develop calibration curves for hemoglobin quantification using Photoacoustic Spectroscopy. For this purpose, human hemoglobin solutions with controlled concentrations were prepared by dilution in saline solution, and their corresponding optical absorption spectra were recorded. The ratios between the optical absorption at 412 nm (γ peak or Soret band) and at 450 nm were calculated and plotted as a function of hemoglobin concentration. These data were then fitted with the most appropriate mathematical function to generate

a hemoglobin calibration curve. This calibration enables the estimation of hemoglobin concentration in various biological systems, such as blood, plasma, urine, and other hemoglobin-containing media. A typical PAS setup used for optical characterization comprises a light source, monochromator, chopper, photoacoustic cell, lock-in amplifier, and computer for data acquisition [28].

In addition to the biomedical relevance of hemoglobin, the calibration curves developed in this study could be applied in other fields requiring precise quantification of proteins or other biomolecules present in the bloodstream or tissues. Integrating these calibration models into clinical equipment could greatly enhance the accuracy of noninvasive hemoglobin measurements, thereby contributing to the advancement of personalized medicine and real-time patient monitoring.

This research represents a step forward in enhancing biomolecule quantification techniques using photoacoustic spectroscopy, with promising implications for diagnostic and therapeutic medicine [29] [29–31].

2 Materials and Methods

2.1 Preparation of Dilutions

To determine hemoglobin concentration in both optically opaque samples (such as blood) and optically transparent samples (such as urine and plasma), two sets of dilutions were prepared, resulting in two corresponding calibration curves.

The dilutions were prepared by mixing human hemoglobin reagent (Sigma-Aldrich) as the solute with isotonic saline solution as the solvent. The first set of dilutions contained high hemoglobin concentrations (20, 40, 80, 100, 120, 140, 160, and 180 mg/mL) and was used to obtain the calibration curve for optically opaque samples. The second set contained low hemoglobin concentrations (0.03175, 0.0625, 0.125, 0.25, 0.5, 1, and 2 mg/mL) and was used to construct the calibration curve for optically transparent samples.

2.2 Characterization by Photoacoustic Spectroscopy

2.2.1 PAS Experimental Setup

The PAS experimental setup used to obtain the optical absorption spectra of the hemoglobin solutions consisted of a 700 W Xe lamp (Oriel) as the light source, a monochromator (Oriel), an optical chopper (Stanford Research Systems), a photoacoustic cell, a lock-in amplifier (Stanford Research Systems), and a computer for data acquisition. The photoacoustic cell was constructed from a brass plate, forming a cylindrical cavity 3 mm in height and 6 mm in diameter. Inside the cavity, a narrow acoustic channel connects the chamber to an electret microphone, which detects the pressure variations generated by the absorption of modulated light by the sample. These periodic pressure oscillations, produced by the photoacoustic effect, are

converted into electrical signals by the microphone, amplified by the lock-in amplifier, and recorded by the computer [28].

2.2.2 Optically Opaque Samples

For the high hemoglobin concentrations corresponding to optically opaque samples, the characterization by PAS was performed in absorption mode. A volume of 60 μL of each dilution was placed inside the photoacoustic cell, and the optical absorption spectrum was recorded over a wavelength range of 250–750 nm. Each measurement was repeated five times for every concentration to ensure statistical reproducibility.

2.2.3 Optically Transparent Samples

For the low hemoglobin concentrations corresponding to optically transparent samples, the configuration of the photoacoustic cell was slightly modified. Unlike the high-concentration samples, which were placed inside the cell, these samples were positioned on the external surface of the quartz window. Graphite powder was placed inside the cell as a reference absorber, and the characterization was performed in transmission mode. In this configuration, 100 μL of each dilution were applied, and the measurements were repeated five times per concentration over a wavelength range of 250–750 nm.

3 Results and Discussion

The optical absorption spectrum of blood, as reported in the literature, exhibits three characteristic peaks. The first peak, located at 412 nm, corresponds to the Soret band or γ peak and arises from the iron present in hemoglobin [32, 33]. The second and third peaks, known as the β (~ 550 nm) and α (~ 580 nm) peaks, are also well documented [34].

The optical absorption spectrum of the Sigma-Aldrich human hemoglobin reagent is shown in Fig. 1. The Soret band is clearly visible, with its maximum absorption at 412 nm, in agreement with previously reported values literature [35]. The β and α peaks, typically located at 550 nm and 580 nm, respectively, are not well defined in this spectrum. This is because the hemoglobin used is in the non-oxygenated form, which is consistent with literature reports [36, 37].

3.1 Optically Opaque Samples (High Concentrations)

As mentioned in the Materials and Methods section, two calibration curves were constructed. The first corresponds to high hemoglobin concentrations (20–180 mg/mL) and can be used to estimate hemoglobin levels in optically opaque samples. The optical absorption spectra obtained for these concentrations are shown in Fig. 2, where all samples exhibit a maximum absorption around 412 nm, corresponding to the γ (Soret) peak associated with the iron in hemoglobin [32, 33]. It is worth

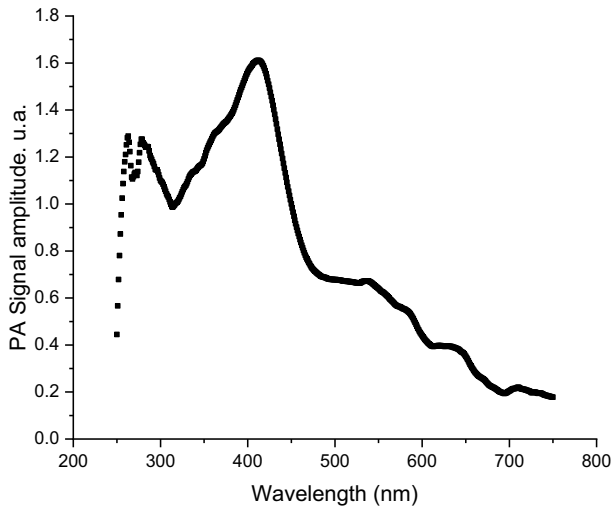


Fig. 1 Optical absorption spectrum of the Sigma-Aldrich human hemoglobin reagent diluted in saline solution

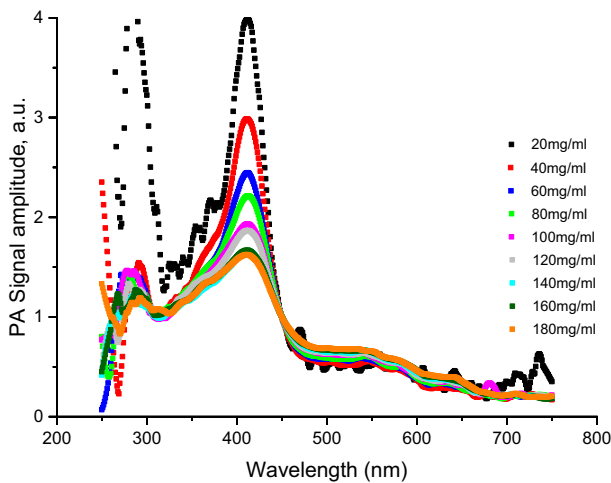


Fig. 2 Optical absorption spectra of hemoglobin solutions at different concentrations, used to construct the calibration curve for optically opaque samples

noting that, although the absorption intensity of the γ peak decreases as the hemoglobin concentration increases, the parameter that indicates whether the concentration is increasing or decreasing is the ratio of the γ peak absorption to that at 450 nm. According to reports in the literature, this ratio is inversely proportional to the hemoglobin concentration [17, 27]. It should be noted that in the literature, the absorption ratio of the γ peak to the β or α peaks is commonly considered; however, in the present study, the ratio of the γ peak absorption to that at 450 nm was used

instead. This choice was made because, in the case of non-oxygenated hemoglobin, such as the one employed in this work, the β and α peaks are not well defined and exhibit significant variation in their absorption, whereas the spectrum at 450 nm is well defined and stable. Figure 2 also shows absorption in the 250–300 nm range. According to previous reports, some components of the saline solution used to dilute the Sigma-Aldrich human hemoglobin reagent exhibit absorption at these wavelengths [38].

3.1.1 Calibration Curves

By taking the ratios of the γ peak to the 450 nm absorption from the spectra of each concentration (20–180 mg/mL), the calibration curve shown in Fig. 3 was obtained. Each concentration was measured five times, yielding five ratio values per concentration, which were plotted as a function of hemoglobin concentration. The best-fitting curve corresponded to an exponentially decreasing function [38], with a correlation coefficient of $R^2 \approx 0.98$ (see Fig. 4). These results confirm the reliability of this method for estimating hemoglobin concentration in optically opaque media [39].

3.1.2 Spectral Area Integration Method (SAIM)

To quantitatively evaluate the variations in the photoacoustic (PA) signal with hemoglobin concentration, the Spectral Area Integration Method (SAIM) was applied. This approach consists of integrating the area under the PA spectrum within a specific wavelength window that includes the main absorption peak of hemoglobin, known as the Soret band, located around 412 nm. For this purpose, the integration

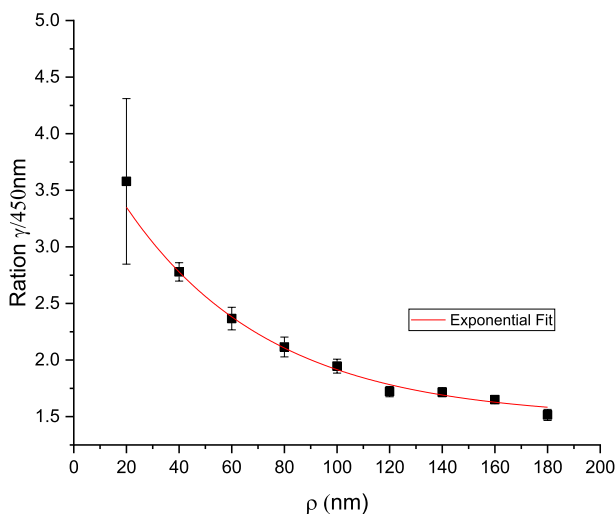


Fig. 3 Calibration curve obtained from the $\gamma/450$ nm absorption ratios, calculated from the optical absorption spectra of hemoglobin solutions with concentrations ranging from 20 mg/mL to 180 mg/mL

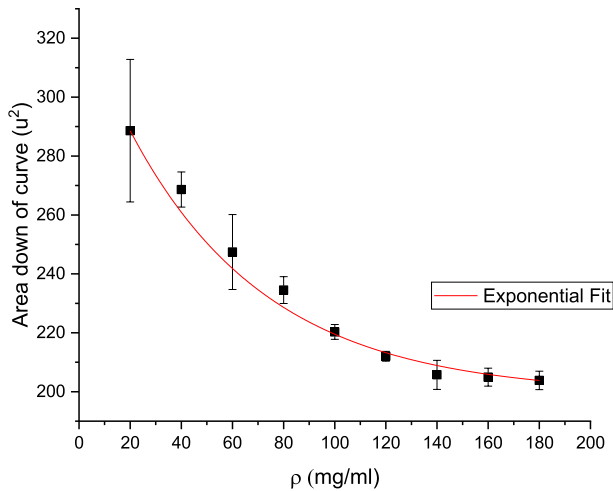


Fig. 4 Integrated area under the spectral curve for different hemoglobin concentrations, used to construct the calibration curve for high-concentration samples

was performed over the range of 315–480 nm, which encompasses the full width of the Soret band while minimizing contributions from adjacent spectral regions. This wavelength window ensures that the calculated area accurately represents the intensity and absorption characteristics associated with hemoglobin. It was observed that the integrated area decreases as hemoglobin concentration increases, reflecting the number of molecules in the sample. These results are consistent with previous reports in the literature [40, 41] (see Fig. 4).

3.2 Optically Transparent Samples (Low Concentrations)

For low hemoglobin concentrations (0.0312–2 mg/mL), the samples are optically transparent, and their characterization was performed in a transmission configuration. The same photoacoustic cell was used for both opaque and transparent samples. For opaque samples, the material was placed inside the hermetically sealed cell, with modulated light incident directly on the sample. In contrast, for transparent samples, the material was positioned on top of the quartz window outside the cell, while a graphite layer (0.0110 g) was placed inside the cavity directly beneath the window. The modulated light passed through the transparent sample and was subsequently absorbed by the graphite, generating the photoacoustic effect within the cell. The optical absorption spectra of these dilutions are shown in Fig. 5. The γ peak (412 nm), associated with the iron in human hemoglobin [32, 33], increases in absorption as the concentration rises; however, as noted previously, the ratio of the γ peak to the absorption at 450 nm is what determines whether the hemoglobin concentration is increasing or decreasing [27]. Similar to the high-concentration samples, an absorption feature is observed in the 250–300 nm region, attributed to proteins and components of the saline solution used for dilution [38].

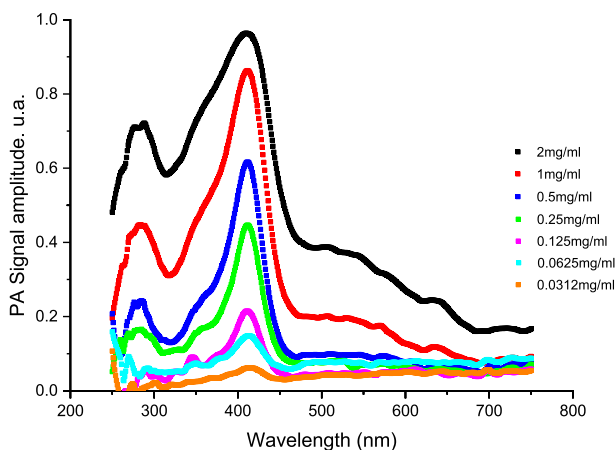


Fig. 5 Optical absorption spectra of hemoglobin solutions at different concentrations, used to construct the calibration curve for optically transparent samples

3.2.1 Calibration Curve

To construct the calibration curve for low-concentration hemoglobin dilutions, optical absorption values were obtained from the transmission spectra. The absorptions at the γ peak and at 450 nm were used to calculate their ratio for each sample. Each concentration was measured five times, and the resulting ratios, along with their statistical estimates, were plotted (Fig. 6). The data were best fitted by an exponentially decreasing function, which accounts for 99 % of the experimental variation. This

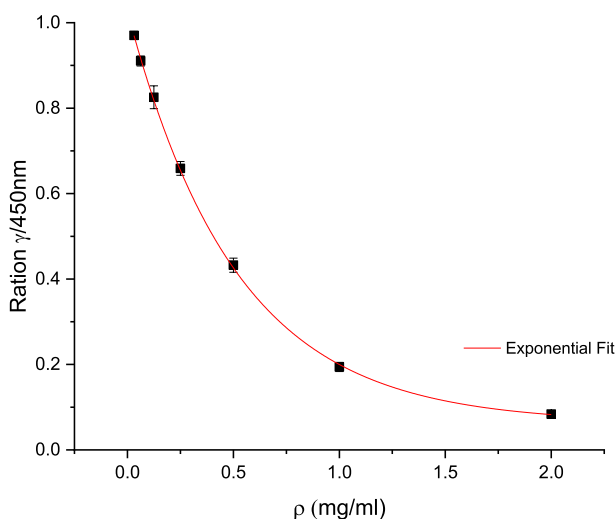


Fig. 6 Calibration curve for low-concentration hemoglobin solutions, corresponding to optically transparent samples

calibration curve allows hemoglobin concentrations in optically transparent samples to be estimated with an approximate margin of error of 1 %.

It is important to note that the calibration curve shown in Fig. 6 was constructed from the normalized transmission spectra, rather than the absorption spectra presented in Fig. 5. This approach was adopted because, for optically transparent samples, the photoacoustic cell operated in transmission mode, with light passing through the sample and being absorbed by a graphite layer inside the cell. All spectra were normalized to 450 nm to minimize variations due to lamp intensity and sample positioning. Using the original transmission data ensured a more consistent and reliable relationship between the γ parameter and the optical response of hemoglobin.

3.2.2 Spectral Area Integration Method (SAIM)

To quantitatively evaluate the spectral changes in low-concentration (optically transparent) samples, the Spectral Area Integration Method (SAIM) was applied. As in the previous section, the integration was performed around the Soret band at 412 nm, which remains detectable even at low optical densities. The integration range was 315–480 nm. It was observed that the integrated area in this region increases with concentration, reflecting the higher number of hemoglobin molecules contributing to absorption [40–42] (see Fig. 7).

The results confirm that Photoacoustic Spectroscopy is a reliable technique for generating hemoglobin calibration curves under varying optical conditions. The correlation between the absorption ratios at 412 nm and 450 nm and hemoglobin concentration enables highly accurate estimates, even when α and β peaks are poorly defined, as is the case for deoxygenated hemoglobin.

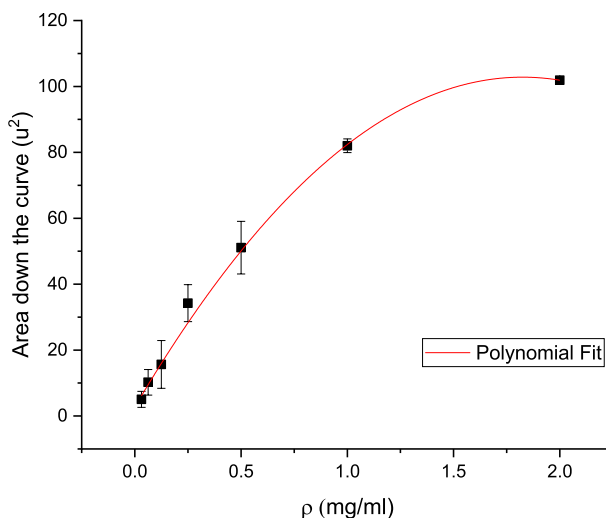


Fig. 7 Integrated area under the spectral curve for different hemoglobin concentrations, used to construct the calibration curve for low-concentration samples

This approach offers several advantages over conventional optical methods, including minimal sample requirements, non-destructive measurement, and applicability to both opaque and transparent media. Moreover, the high reproducibility observed ($R^2 > 0.98$ in both cases) indicates that the calibration curves obtained could be readily implemented in clinical devices for rapid, noninvasive hemoglobin determination in biological fluids.

4 Conclusion

In this work, hemoglobin calibration curves were developed using Photoacoustic Spectroscopy under two experimental conditions: optically opaque and transparent solutions. In both cases, the absorption spectra consistently exhibited the Soret band, with a peak at 412 nm, and the 412/450 nm spectral ratio proved to be a reliable parameter for the quantitative estimation of hemoglobin concentration. The obtained calibration curves exhibited high correlation coefficients ($R^2 > 0.98$), validating the reliability of the method across a wide range of concentrations. Additionally, the Spectral Area Integration Method (SAIM) confirmed the expected concentration-dependent trends, consistent with previous reports. A comparison between the two analytical approaches—the $\gamma/450$ nm absorption ratio and SAIM—indicates that both can effectively quantify hemoglobin concentrations using PAS. However, under the experimental conditions of this study, SAIM demonstrated greater sensitivity and stability, particularly at low concentrations where the signal-to-noise ratio is limited. This improved performance arises from SAIM's integration of the full spectral contribution within the Soret band region (315–480 nm), which reduces the impact of local fluctuations in the photoacoustic signal or variations in lamp intensity. In contrast, the $\gamma/450$ nm ratio method, based on the relative intensity between two wavelengths, is more susceptible to minor alignment or optical power variations. Therefore, SAIM provides a more robust and reliable analytical parameter for evaluating the photoacoustic response of hemoglobin samples under the conditions analyzed.

These results underscore the sensitivity and precision of PAS compared to the limitations of conventional optical techniques. Overall, the findings demonstrate that PAS is a reliable and versatile method for hemoglobin quantification in biological media. Its noninvasive nature, minimal sample requirements, and adaptability to diverse optical conditions highlight its potential for clinical diagnostics and biomedical research. Future studies should focus on *in vivo* validation and the integration of these calibration curves into clinical monitoring systems.

Supplementary Information The online version contains supplementary material available at <https://doi.org/10.1007/s10765-025-03686-3>.

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administration, funding, writing, and review. Guadalupe Cleva Villanueva participated through the management of a project for the management of equipment and materials.

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Data Availability The datasets generated and/or analyzed during the current study are available from the corresponding author upon reasonable request **. **

Declarations

Competing Interests The authors declare no competing interests.

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